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Review Paper

History of Mathematical-Chemistry in Iran: Scientific works of Alireza Ashrafi

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Abstract. The field of mathematical chemistry started with the pure and memorable activities of Alireza Ashrafi in Iran. One of the most important factors in the rapid expansion of this branch of science in Iran, which intensified almost since 2003, has been the regular holding of mathematical chemistry conferences in Iran which were the Iranian version of MCC conferences in Europe. One of the prominent features of Ashrafi was his active and effective presence in international scientific communication and diplomacy, and at the same time holding an international conference on mathematical chemistry in Iran. With his invitation, many scientists from all over the world came to Iran and scientific diplomacy in his field of expertise became popular in the real sense. The mathematical chemistry conferences in Iran were a series of academic conferences that focused on the intersection of mathematics and chemistry. These conferences have been held annually since 2005 and were organized by prominent Iranian mathematicians and chemists, including Alireza Ashrafi and Ali Iranmanesh. The conferences brought together researchers, professors, and students from Iran and around the world to discuss topics such as chemical graphs, topological indices, and mathematical modelling of chemical systems. These conferences have helped to promote the development of mathematical chemistry in Iran and have facilitated collaborations between Iranian and international researchers. The conferences have also produced numerous publications in top scientific journals and have helped to establish Iran as a leading country in the field of mathematical chemistry. In this paper, we focus

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on Ashrafi's work and his co-authors who are pioneers in mathematical chemistry in Iran.

1 Introduction

The origins of mathematical chemistry can be traced back to the 18th century, as demonstrated by Mikhail Lomonosov's "Elementa Chimiae Mathematicae," published in 1741 as documented in. This work served as an early attempt at mathematically formalizing chemistry. Lomonosov's manuscript, titled "Elementa Chimiae Mathematicae," was written in Latin in 1741 and was intended to serve as an introduction to a planned comprehensive chemical treatise that aimed to present all existing chemical knowledge in a systematic and axiomatic manner. However, this project had to be abandoned due to its premature nature, as Lavoisier had not yet been born at the time [141]. However, the formal application of mathematics beyond simple arithmetic and chemical stoichiometry in chemistry dates back to the 19th century and the work of Crum Brown. The term mathematical chemistry itself is relatively new, and it is believed that it first appeared in a paper by John Hasbrouck Van Vleck published in 1928, see [141]. Discrete mathematics entered chemistry through structural theory, initially including graph theory and later topology and group theory. Graph theory is linked to constitutional formulae, which represent chemical, constitutional, or molecular graphs. The totality of information about connectivity in molecular graphs is referred to as molecular topology, although it has little in common with modern-day topology. Group theory is an appropriate mathematical framework for formalizing symmetry, which is important in almost every area of chemistry.

In mathematical chemistry, topological indices are numerical parameters calculated based on the molecular graph of a chemical compound. These indices characterize the topology of a graph and are used to develop quantitative structure-activity relationships (QSARs), which correlate biological activity or other properties of molecules with their chemical structure. Topological indices are numbers applied to a graph that describe specific graph properties through algebraic structures. Algebraic graph theory is a helpful tool in various chemistry domains, [128].

Mathematical chemistry [124] is the area of research engaged in novel applications of mathematics to chemistry; it concerns itself principally with the mathematical modelling of chemical phenomena, see [77]. Mathematical chemistry has also sometimes been called computer chemistry, but should not be confused with computational chemistry.

In the field of mathematical chemistry, a topological index, also known as a connectivity index, is a type of molecular descriptor that is calculated based on the molecular graph of a chemical compound, see [124]. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure, see [77].

In other words, topological indices are numbers that are applied to a graph and can be

used to describe specific graph properties through algebraic structures. Algebraic graph theory is a helpful tool in a range of chemistry domains.

Simultaneously with the growth of the branch of mathematical chemistry in the world, this branch of science also expanded in Iran, and the first mathematician who published articles in this field was professor Seyed Alireza Ashrafi, [4–7].

In other words, the first paper in the field of mathematical chemistry by an Iranian mathematician was published in 2003, authored by Alireza Ashrafi and Masoud Hamadanian, see [79]. Titled "The full non-rigid group theory for tetraamino platinum(II)", the paper utilized finite method theory to obtain results. While the paper primarily focused on molecular symmetry groups, it holds significance as the first article published by an Iranian mathematician in the field of chemistry, despite numerous publications by chemists before it. Following its publication, Hamadanian and Darafsheh co-authored several articles until 2005, [25–27] as well as [43–45]. Later Ashrafi, Iranmanesh, Ghorbani and Taeri continued, computing of topological indices based on symmetry group, see [3, 40, 41, 60–63, 67, 83, 86, 88, 129].

The initial publication by Iranmaneshet al. in 2005 titled "The full non-rigid group theory for the bipyramidal geometry of pentamethylphosphorus" published by MATCH in 2005 [40] and the joint paper by Ghorbani and Ashrafi in 2006, titled "Symmetry of tetrashydroxycalix [4] arenes", appeared in the journal of Serbian Chem. Soc. Prior to this, Ashrafi had contributed to the field of group theory and published articles about Cayley graphs. It is worth mentioning that there were earlier submissions to journals that were published after 2006.

In 2008, the duo published their first article in the field of bio-mathematics, entitled "Computing orbits of the automorphism group of subsequence poset", in the journal Order, see [66]. Ashrafi expressed his conviction that bio-mathematics would gain widespread popularity both in Iran and worldwide in the near future. Under their guidance, several senior students also worked on topics related to DNA structure and graphs, resulting in two published articles, in which Farhami was a co-author in both articles [17, 53].

Furthermore, Alireza Ashrafi and Amir Loghman [31] published the first paper on chemical graph theory without any trace of group theory in 2004. The paper, titled "PI Index of Zig-Zag Polyhex Nanotubes", is noteworthy for utilizing graph theory techniques to calculate topological indices, as Ashrafi had previously been interested in calculating the self-alignment group or symmetry group of molecules. The paper has been referenced 164 times in Google Scholar and has became the favourite topic of many mathematicians and mathematics students in Iran.

In 2005, Ashrafi collaborated with Mohammadreza Ahmadi [8] on an article titled "New computer program to calculate the symmetry of molecules", and published further articles in this field with Vakili-Nezhaad and Moghani, see [33] as well as [9, 18, 20–22, 28–30, 116–120]. Ashrafi co-authored or edited 21 book chapters and six books with other Iranian authors [1,2,10–16,23,24,35,37–39,50,64,72–76,81,82,121–123]. He was also the founder and long-time Editor of "Iranian Journal of Mathematical Chemistry". The existence of IJMC (third mathchem journal worldvide) is of great importance for Iranian mathematical chemistry [87].

It is interesting to see how the field of chemical graphs and their topological indices at-

Figure 1. From the right: Ivan Gutman, Gholamhossein Fath-Tabar, Alireza Ashrafi, 4th Conference and Workshop in Mathematical Chemistry, Dezful Azad University, Dezful, February 5–6, 2011.

tracted a lot of attention from various researchers and scholars. It is also noteworthy that the interest in this field continued to grow, as more people joined the group and more students were trained to conduct research in this area.

Topological indices have proven to be valuable tools in the field of chemistry, as they provide information about the structure and properties of molecules. By using these indicators, researchers can gain insights into the behavior of molecules and predict their chemical and physical properties, [48, 49, 52, 68] as well as [124, 126, 127, 142–144].

It is clear that the work of these researchers has contributed significantly to the development of the field of chemical graphs and topological indices. Their efforts have helped to expand our understanding of the structure and behavior of molecules, and they continue to inspire new research and discoveries in this area, [55–59, 89, 101–115].

After the PI index, which first caught Ashrafi's attention, the Wiener index became the focus of his collaborative work with Yousefi-Azari and Khalifeh [90–99, 145–148, 150]. They, along with Shahram Yousefi and Behzad Manoochehrian published several articles on this topic, with the detour index following soon after [32, 149]. Gradually, their work shifted from ordinary graphs to chemical graphs. The good cooperation between Iranmanesh and Ashrafi and their effective communication with Professor Ivan Gutman from Serbia, the editor of the famous MATCH journal, and a prominent figure in the field, led to many Iranian articles being published in the magazine, Gutman, along with Alexander Balaban, Ante Graovac, Harou Hosoya, Milan Randić, and Nenad Trinistić are known as a pioneer in mathematical-chemistry. Gutman visited Iran many times, and after each lecture, he usually presented on a particular index, leading to a large number of professors and students researching the topic not only in Iran but worldwide.

It's great to hear that the cooperation with world-class scientists through international conferences led to the idea of holding mathematical chemistry conferences by Ashrafi and

Figure 2. From the right: Mohammad Hassan Khalifeh, Modjtaba Ghorbani, Mohammad Ali Salahshour, Alireza Ashrafi, Gholam Hossein Fath-Tabar, Mircea Diudea, Farzane Gholami-Nezhaad, Mahsa Mirzargar and Asefeh Karbasioun. The First Confrence and Workshop on Mathmatical Chemistry, Tarbiat Modares University, Tehran January 29–31, 2008.

Iranmanesh. The collaboration with Ivan Gutman and Ante Graovac is also commendable. It's wonderful to know that the first mathematical chemistry conference was held in Iran and was hosted by Tarbiat Modares University. Ali Iranmanesh was the chair of that conference. Such conferences can bring together experts from different parts of the world to share their knowledge and research findings, leading to the advancement of science and technology, see [34, 51, 65, 70, 78, 80, 84, 85, 100].

The participation of well-known scientists from different countries in the mathematical chemistry conferences held in Iran played a crucial role in introducing new ideas and approaches to chemical graph theory and its applications. The impact of these conferences and collaborations can be seen in the significant contributions made by Iranian researchers, such as Nadjafi-Arani, in advancing the field of chemical graph theory and its applications, particularly in the Wiener index.

Ashrafi in [54] says: "In the world Mathematical Year (WMY 2000), the Shahid Beheshti University at Tehran organized an inaugural meeting for the heads of mathematics departments of the country. In the end of meeting the representative of the Ministry of Culture and Higher Education (MCHE) announced that the country needs some experts in mathematical chemistry. I (ARA) participated in this meeting and decided to start working on the subject. The papers by Smeyers and his co-authors leaded me to choose Chemical Group Theory mostly in the topic of "symmetric groups of molecules" for the first attempt. The first work on the subject in the country was related to our first collaboration with Ante."

Gutman in [71] says "Soon we got in touch, soon we started to do joint research, soon Ali Reza became member of Editorial Board of our "MATCH Communications in Mathematical and in Computer Chemistry" (where he published a total of 43 contributions). Eventually, we met on many mathematical chemistry conferences held in Iran, when I experienced the unforgettable Iranian hospitality. We also met on a couple of conferences in Dubrovnik, Croatia, on one of which Ali Reza was elected member of the International Academy of Mathematical Chemistry (to what I contributed a bit)." After the successful holding of the first course in Tar-

Figure 3. Seated from right: Ivan Gutman, Sandy Klavzar, Mircea Diudea, Ante Graovac. Standing from the right: Alireza Ashrafi and Ali Iranmanesh. The First Confrence and Workshop on Mathmatical Chemistry, Tarbiat Modares University, Tehran January 29–31, 2008.

biat Modares University and the great reception of those interested in this field, the second and third mathematical chemistry conferences were held in Kashan and Tarbiat Modares universities, respectively, and the number of people interested in this field of science is increasing day by day. The variety of people who were invited from different countries had a significant contribution to the expansion of this branch of science. In the second conference, professor Michael Deza from France was also present. He was a Russian-French mathematician who specialized in combinatorics, geometry, discrete and graph theory. He was Director Emeritus of Research at the French National Center for Scientific Research (CNRS), Vice-Chancellor of the European Academy of Sciences, research professor at the Advanced Institute of Science and Technology of Japan, and Editor-in-Chief of the renowned European Journal of Combinatorics. Among the other invitees of this conference were Professor Tomislav Došlić from Croatia along with Gutman, Diudea and Graovac.

Collaborating with European professors and publishing joint articles is a great way to advance scientific research and knowledge. It's great to see that Ashrafi was one of the main authors in most of these articles and that he was able to work with his colleagues and students to achieve significant results in this field.

The third mathematical chemistry conference was again hosted by Tarbiat Modares University and the same group of attendees from the previous conferences was present. During this time, Hassan Khalifeh, a former student of Yousefi-Azari at the University of Tehran, had become a prominent figure in the field. He had co-authored several articles related to distance in graphs with Ashrafi and Yousefi-Azari and had successfully solved several previously unsolved problems, see [90–99]. Additionally, Heydari and Arezoomand [3, 129] from Isfahan had also published articles in this area, indicating the rapid expansion of this field in Iran. Ghorbani had the pleasure of attending all of these conferences and was invited to speak at each event. In fact, the speech of Ghorbani at the third mathematical chemistry con-

Figure 4. The Second Iranian Conference and Workshop on Mathematical Chemistry, University of Kashan, Kashan, April 14–16, 2009.

Figure 5. The Third Iranian Conference and Workshop on "Mathematical Chemistry" Tarbiat Modares University, Tehran, February 22–24, 2010.

ference at Tarbiat Modares University was honoured as the best speech of the conference. The relationships between Iranian scientists with prominent European professors were strengthened over time and they published many joint articles with them. In most cases, Ashrafi was one of the main authors and typically worked with other students or colleagues.

At Ghorbani's invitation, Diudea came twice to Shahid Rajaee Teacher Training University (SRTTU) and gave several lectures in the field of mathematical chemistry. During his

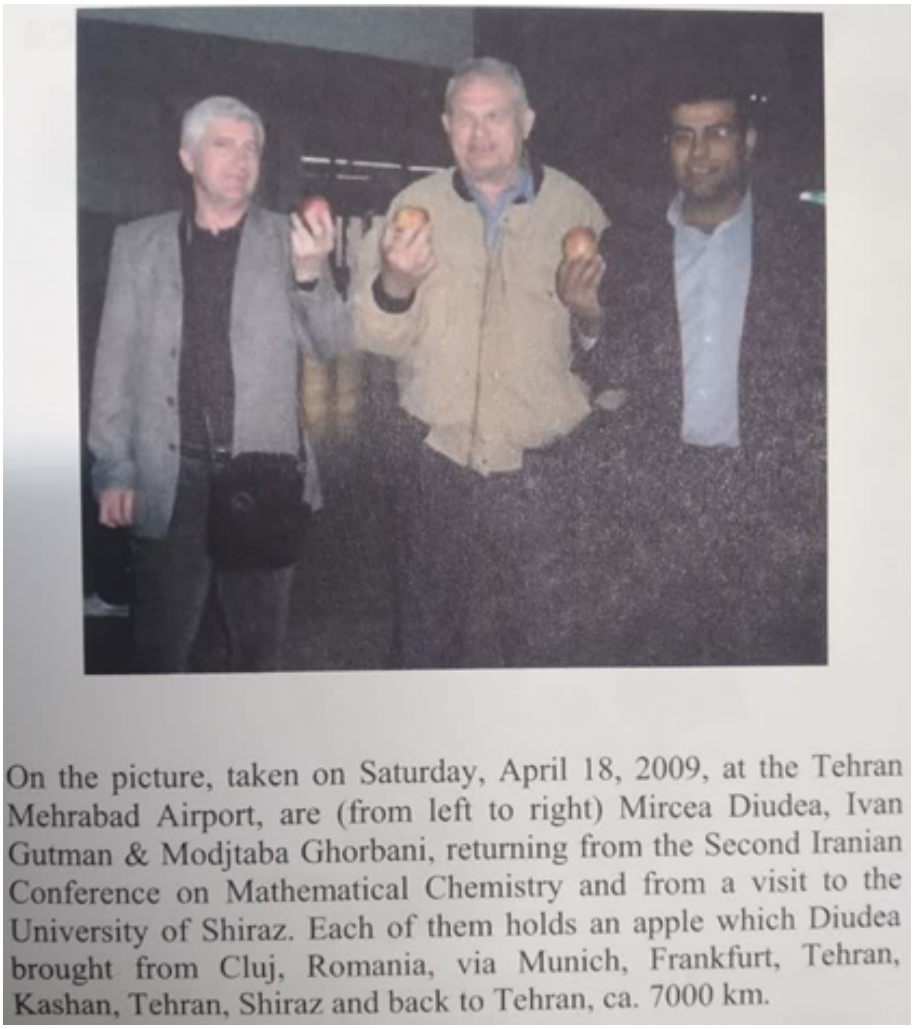

Figure 6. The 2nd Iranian Mathematical-Chemistry Conference and Workshop, from a visit to the University of Shiraz.

first visit to SRTTU, which coincided with the second mathematical chemistry conference, he talked to the Persian participants for a few minutes and surprised everyone. As a 7th language, he also spoke Persian and had become so proficient that he could understand Farsi but could hardly speak it. He had a lot of scientific cooperation with Iranians and happy memories of that time have been left. Prof. Ashrafi explained, once he was speaking at a conference in Europe and a chemist told him that your results are mathematically correct but chemically wrong. He was saying that someone gently patted my back and said that if you want, I can help you and we became friends very soon, see [61]. He was none other than Mircea, who was a lovable and noble person in the true sense of the word. Diudea was struggling with cancer at the end of his life and therefore died very soon.

The first Persian book in the field of mathematical chemistry was published by Bahrami, Yousefi and Ashrafi under the title Nanocomputing and Fullerenes. The second book was published by Iranmanesh, Ashrafi, Loghman and Soleimani under the title of Padmakar-Ivan

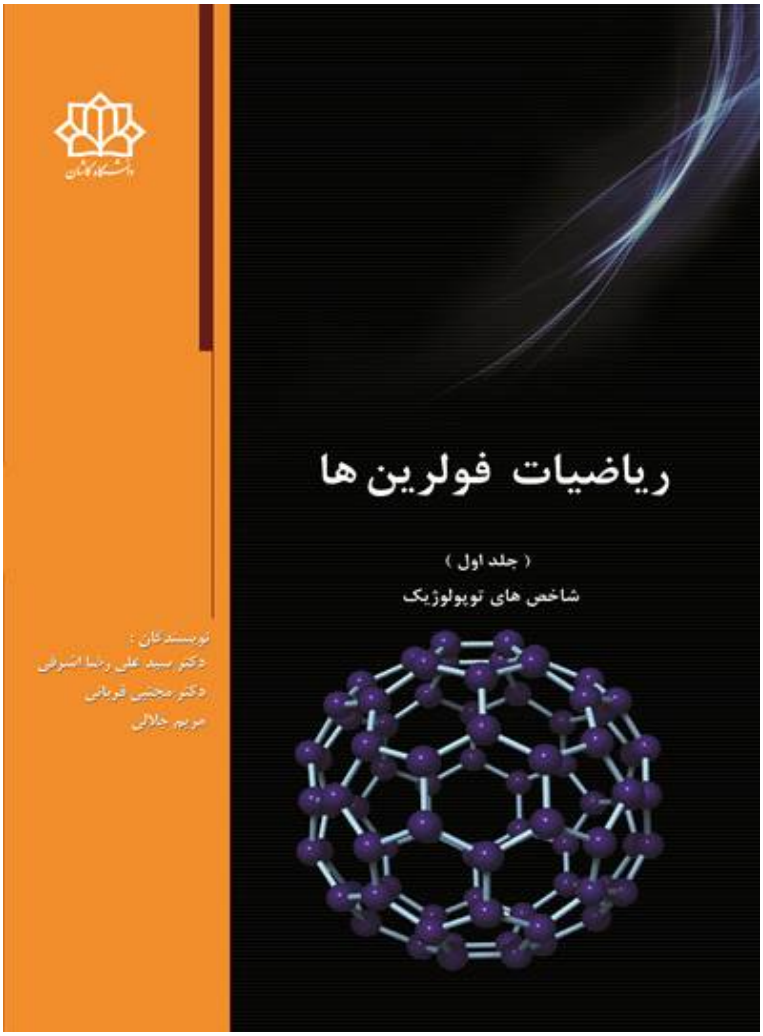

Figure 7. The third book Mathematical Chemistry era in Iran, its title is "Mathematics of Fullerenes".

Index of Nano Tubes and Nano-Torus. The third book was published by Ghorbani, Ashrafi and Jalali in collaboration with Kashan University Press and Soroush Danesh, entitled Mathematics of Fullerenes, which also attracted Ivan Gutman's admiration. This is a two-volume book. In the first volume, well-known topological indices are introduced, and in the second volume, fullerenes are investigated using the techniques of algebraic graph theory and finite group theory.

Ashrafi played the main role in the compilation of all these books and he contributed a lot to the expansion of this branch of science in Iran.

Later, a book with the same title, namely, "Mathematics and Topology of Fullerenes" was published by Springer Publishing, in which Iranians, including Ashrafi, played a key and important role in writing this book. Most importantly for us, Harry Kroto, a Nobel medalist, wrote the introduction to this book. He shared the 1996 Nobel Prize in Chemistry with Robert Curl and Richard Smalley for their discovery of fullerenes. Ghorbani, Ashrafi and Diudea wrote the first chapter of this book. Ghorbani has participated twice in international

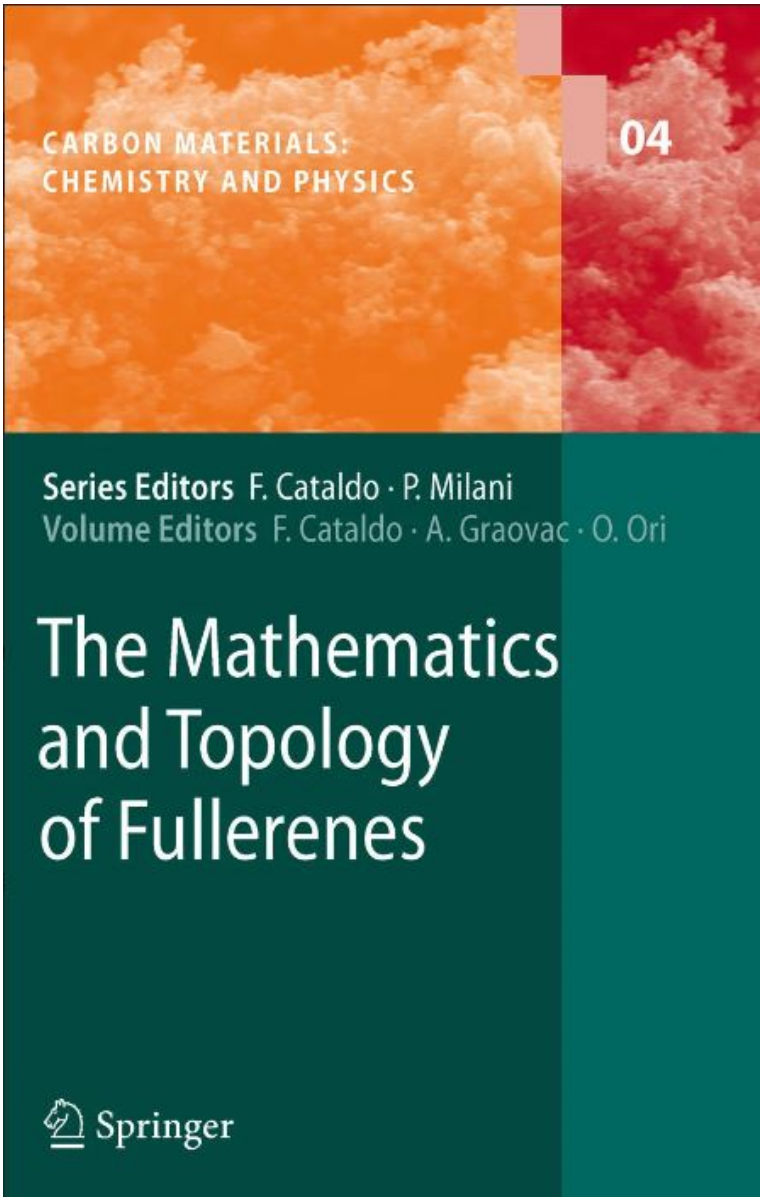

Figure 8. Kroto wrote the preface of the book entitled "Mathematics and Toplogy of of Fullerenes" which is published in 2011, Editors of this book include Franco Cataldo, Ante Graovac,and Ottorino Ori.

conferences on Mathematical Chemistry, the first of which was in 2011, which was held in Dubrovnik, Croatia. Ashrafi and Ghorbani had a meeting with Kroto for several hours. They discussed the problem of the Persian mathematics of the fullerenes book with Kroto. He promised that if a book with this name was written, he would write the introduction to it. This book was finally published with the great efforts of Ashrafi and the late Ante Graovac under the name "Mathematics and Topology of Fullerens" and Kroto wrote the preface of the book as promised. Many Iranians contributed to that book, except for Ashrafi and his students, Iranmanesh and his students also played a leading role in it.

Almost all the Iranians present at the conference also came and there, we took many

Figure 9. From the right: Kroto, Ghorbani and Ashrafi.

souvenir photos with Ashrafi and other friends.

Of course, Ashrafi and Ghorbani also wrote another book about nanostructures and their introduction. In this book, they investigated counting polynomials, the most important of which was the Omega polynomial. This concept was defined by Mircea Diudea and has found many applications in chemistry, especially modelling and calculating the electrovalence energy of nanostructures. Ghorbani invited Mircea to take a souvenir photo with this book and he accepted. Ghorbani immediately called Ashrafi and told him about it. Ashrafi also agreed to take a photo as a souvenir. He was always smiling in all these photos, and he was truly unique in scientific trips and enjoyed everyone.

Between 2008 and 2018, many conferences and seminars were held in Iran on the subject of mathematical chemistry or similar, see [130–140]. One of them was the conference on chemical graph theory, which was organized by the mathematics department of Shahid Rajaee University. The scientific chair of them was Modjtaba Ghorbani and these conferences were held three times in Iran. It was held twice in Rajaee University in the period 2010-2013 [131, 133] and once in Hamedan city [135]. Many mathematicians were invited to these conferences, the most important of whom were Dragos Cvetković, Damir Vukicevic, Bo Zhou and Haro Hosoya, who came to Iran for the first time.

Figure 10. Iranian Scientist that participated at MCC 2011. Standing from right: Ali Iranmanesh, Mohammad Ali Iranmanesh, Hassan Yousefi-Azari, Alireza Ashrafi and Modjtaba Ghorbani. Seated from the right: Morteza Faghani and Gholamhossein Fath-Tabar.

Figure 11. Standing from left; A. R. Ashrafi, M. Diudea and M. Ghorbani

Figure 12. The First Iranian Conference on Chemical Graph Theory, Shahid Rajaee Teacher Training University, Tehran, October 6–7, 2010.

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